

A finite-dimensional representation of the quantum angular momentum operator

(Short title: Angular momentum in a finite linear space)

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Abstract

A useful finite-dimensional matrix representation of the derivative of periodic functions is obtained by using some elementary facts of trigonometric interpolation. This $N \times N$ matrix becomes a projection of the angular derivative into polynomial subspaces of finite dimension and it can be interpreted as a generator of discrete rotations associated to the z -component of the projection of the angular momentum operator in such subspaces, inheriting thus some properties of the continuum operator. The group associated to these discrete rotations is the cyclic group of order N .

Since the square of the quantum angular momentum L^2 is associated to a partial differential boundary value problem in the angular variables θ and φ whose solution is given in terms of the spherical harmonics, we can project such a differential equation to obtain an eigenvalue matrix problem of finite dimension by extending to several variables a projection technique for solving numerically two point boundary value problems and using the matrix representation of the angular derivative found before. The eigenvalues of the matrix representing L^2 are found to have the exact form $n(n+1)$, counting the degeneracy, and the eigenvectors are found to coincide exactly with the corresponding spherical harmonics evaluated at a certain set of points.

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1. Introduction

A Galerkin-collocation-type method based in a N -dimensional matrix representation of $\frac{d}{dx}$ obtained through Lagrange's interpolation has been used to solve one-dimensional boundary value problems (see Refs. [1]–[4]). This technique consists basically in the substitution of the variable x and the derivative $\frac{d}{dx}$ by $N \times N$ matrices X and D in a certain form of the given differential equation. The diagonal matrix X has the N different values x_j , $j = 1, 2, \dots, N$ along the main diagonal, and the matrix D is given by

$$(1) \quad D = P\tilde{D}P^{-1},$$

where

$$(2) \quad \tilde{D}_{ij} = \begin{cases} \sum_{l=1}^N \frac{1}{(x_i - x_l)}, & i = j, \\ \frac{1}{(x_i - x_j)}, & i \neq j, \end{cases} \quad P_{ij} = p'(x_i) \delta_{ij}, \quad i, j = 1, 2, \dots, N,$$

The symbol \sum' appearing in (2) means the sum over $l \neq i$ and the prime on p means differentiation of the polynomial

$$p(x) = \prod_{k=1}^N (x - x_k).$$

The N nodes x_j can be chosen by imposing a condition where the coefficients of the differential equation and the boundary conditions play the main part. This condition is

$$(3) \quad \sum_{k=1}^N \frac{1}{(x_j - x_k)} = -\frac{\gamma'(x_j)}{\gamma(x_j)}, \quad j = 1, 2, \dots, N,$$

where $\gamma(x)$ is a function defined by the boundary conditions and the differential equation (see Refs. [4]–[5]).

More precisely, the projection scheme for the k -th derivative of a real function f evaluated at different (but otherwise arbitrary) points $x_i, i = 1, 2, \dots, N$ is given by

$$(4) \quad f^{(k)}(x_j) = \sum_{l=1}^N D^k_{jl} f(x_l) + E_j, \quad j = 1, 2, \dots, N,$$

where E_j is the j -th component of the residual vector depending on f , N and k . Let us denote by π_{N-1} the space of polynomials of degree at most $N - 1$. Thus, if $f \in \pi_{N-1}$, it is found that (4) is exact at the nodes, *i.e.*, $E_j = 0$, and therefore, any differential problem closed in π_{N-1} can be solved also in \mathbb{R}^N as a matrix problem yielding the same solution. An estimate of the error E_j for other kind of functions is given in [4].

The formal application of this elementary technique to some multivariate problems is straightforward, as shown in the following section (see also [6]).

2. Multivariate case

To illustrate how this method should be applied to some boundary value problems in several variables we will take first two real variables, x and y .

Let $\tilde{\Pi} = \pi_{M-1} \otimes \pi_{N-1}$ be the space of bivariate tensor-product polynomials of degree $N - 1$ in the variable x and $M - 1$ in y . Thus, if $f \in \tilde{\Pi}$, $f(x, y)$ can be written as

$$(5) \quad f(x, y) = \sum_{j=0}^{N-1} \sum_{k=0}^{M-1} a_{jk} x^j y^k.$$

Now let us take two sets of different but otherwise arbitrary points $\{x_1, x_2, \dots, x_{N_1}\}$ and $\{y_1, y_2, \dots, y_{N_2}\}$, on the x and y axes respectively, and let D_x and D_y be the $N \times N$ and $M \times M$ matrix representations of $\frac{d}{dx}$ and $\frac{d}{dy}$ constructed according to (1) with such sets.

By deriving partially (5) n times with respect to x and m times with respect to y , and evaluating the result at the cartesian nodes (x_j, y_k) we obtain the vector $\mathbf{f}^{(n,m)}$ of dimension $\tilde{N} = NM$ whose entries are given by

$$f_r^{(n,m)} = \frac{\partial^{n+m} f(x, y)}{\partial x^n \partial y^m} \Big|_{(x_j, y_k)}$$

where the indexes r, j and k are related through

$$(6) \quad r = j + (k - 1)N, \quad j = 1, 2, \dots, N, \quad k = 1, 2, \dots, M,$$

in such a form that $r = 1, 2, \dots, \tilde{N}$. It is known that a bivariate interpolation on the grid (x_j, y_k) is uniquely possible in $\tilde{\Pi}$ (see [7]) so that f can be taken as a bivariate and sufficiently differentiable real function other than a polynomial, and (5) as its corresponding (tensor) Taylor polynomial. By choosing j (the x -index) to run faster than k and using (4) according to the case, we can write down a matrix formula in $\mathbb{R}^{\tilde{N}}$ for $\mathbf{f}^{(n,m)}$ in terms of $\mathbf{f} = \mathbf{f}^{(0,0)}$, generalizing (4):

$$(7) \quad \mathbf{f}^{(n,m)} = (D_y^m \otimes D_x^n) \mathbf{f} + \mathbf{E}.$$

Here, the Kronecker product of matrices $A = (a_{jk})$ and $B = (b_{jk})$ of sizes $N \times N$ and $M \times M$, respectively, is defined by

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots & a_{1,N}B \\ a_{21}B & a_{22}B & \cdots & a_{2,N}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{N,1}B & a_{N,2}B & \cdots & a_{N,N}B \end{pmatrix}.$$

The components of the residual vector \mathbf{E} are zero if $f \in \tilde{\Pi}$ and an expression for them is given in [8] for sufficiently differentiable functions.

Let 1_x and 1_y denote the identity matrices of dimension N and M respectively, and define the $\tilde{N} \times \tilde{N}$ matrices \mathbf{D}_x and \mathbf{D}_y by

$$(8) \quad \mathbf{D}_x = 1_y \otimes D_x, \quad \mathbf{D}_y = D_y \otimes 1_x.$$

Due to the properties of the Kronecker product, these matrices commute:

$$\mathbf{D}_x \mathbf{D}_y = \mathbf{D}_y \mathbf{D}_x = D_y \otimes D_x.$$

More generally,

$$\mathbf{D}_x^n \mathbf{D}_y^m = (1_y \otimes D_x^n)(D_y^m \otimes 1_x) = D_y^m \otimes D_x^n,$$

and therefore, (7) takes the form

$$(9) \quad \mathbf{f}^{(n,m)} = \mathbf{D}_x^n \mathbf{D}_y^m \mathbf{f} + \mathbf{E},$$

indicating that the partial derivatives $\partial/\partial x$ and $\partial/\partial y$ take in $\tilde{\Pi}$ the tensor-product forms given in (8).

By using the properties of the tensor product and defining $\mathbf{P} = P_y \otimes P_x$ and

$$\tilde{\mathbf{D}}_x = 1_y \otimes \tilde{D}_x, \quad \tilde{\mathbf{D}}_y = \tilde{D}_y \otimes 1_x,$$

where P_x, P_y, \tilde{D}_x and \tilde{D}_y have the structure given in (2), it is possible to give the following alternate form of (9):

$$\mathbf{f}^{(n,m)} = \mathbf{P} \tilde{\mathbf{D}}_x^n \tilde{\mathbf{D}}_y^m \mathbf{P}^{-1} \mathbf{f} + \mathbf{E}.$$

On the other hand, the projection of the coefficient functions of the differential operator can be written as diagonal matrices since the the product of a function $a(x, y)$ by the partial derivatives of the unknown function evaluated at the nodes (x_j, y_k) is

$$a_r f_r^{(n,m)} = a(x_j, y_k) f^{(n,m)}(x_j, y_k)$$

($a(x_j, y_k)$ should be well defined) and the indexes can be ordered according to (6), producing that in this scheme, the coefficient functions can be represented by $\tilde{N} \times \tilde{N}$ diagonal matrices whose non-zero elements are given by $a_r = a(x_j, y_k)$, where r, j and k are related by (6). Let us denote this generic coefficient matrix by

A. Thus, the part of the differential operator consisting in the product $a(x, y)f^{(m,n)}(x, y)$ takes the matrix form

$$\mathbf{A} \mathbf{D}_x^m \mathbf{D}_y^n \mathbf{f}.$$

If $a(x, y)$ accept a Taylor expansion (this condition is too restrictive and it can be relaxed, but it is adequate for our illustrative purposes), we have that **A** can be defined by the same function $a(x, y)$ through

$$\mathbf{A} = a(\mathbf{X}, \mathbf{Y}),$$

where **X** and **Y** are the matrices given by

$$\mathbf{X} = \mathbf{1}_y \otimes X, \quad \mathbf{Y} = Y \otimes \mathbf{1}_x,$$

where the $N \times N$ diagonal matrix X has the set of points x_j , $j = 1, 2, \dots, N$ along the main diagonal whereas the M points y_j lie along the main diagonal of the $M \times M$ matrix Y . **X** and **Y** represent the variables x and y , respectively.

The generalization to the case of q variables x_1, x_2, \dots, x_q is straightforward. We will choose N_j points on the x_j -axis, and the projection space as the tensor product of the subspaces of polynomials of degree at most $N_j - 1$ in x_j , *i.e.*,

$$\tilde{\Pi} = \bigotimes_{j=1}^q \pi_{N_j-1}.$$

The nodes will be ordered in such a way that a function $f(x_1, \dots, x_q)$ evaluated at the nodes yields the vector **f** whose entries are

$$f_r = f(x_{j_1}^1, x_{j_2}^2, \dots, x_{j_q}^q), \quad j_k = 1, 2, \dots, N_k, \quad k = 1, 2, \dots, q,$$

and the indexes r and j_k are related through

$$r = j_1 + (j_2 - 1)N_1 + (j_3 - 1)N_1N_2 \dots + (j_q - 1)\tilde{N}/N_q, \quad j_k = 1, 2, \dots, N_k, \quad k = 1, 2, \dots, q,$$

and $\tilde{N} = \prod_{k=1}^q N_k$. The index than runs faster is j_1 , then j_2 and so on, yielding that $r = 1, 2, \dots, \tilde{N}$.

The $\tilde{N} \times \tilde{N}$ matrix representation of $\partial/\partial x^k$, is now

$$\mathbf{D}_k = \mathbf{1}_q \otimes \dots \otimes \mathbf{1}_{k+1} \otimes D_k \otimes \mathbf{1}_{k-1} \dots \otimes \mathbf{1}_1,$$

where $\mathbf{1}_j$ is the $N_j \times N_j$ identity matrix and D_k is a matrix of dimension N_k having the structure given by (1). Similarly, the representation of the variable x^k is

$$\mathbf{X}^k = \mathbf{1}_q \otimes \dots \otimes \mathbf{1}_{k+1} \otimes X^k \otimes \mathbf{1}_{k-1} \dots \otimes \mathbf{1}_1.$$

In the next section we adapt this technique to other kind of subspaces and it will be applied to an important physical problem in Section 4.

3. Discrete rotations

In this section we show that a matrix representation of the angular derivative (the derivative of univariate periodic functions), can be related to a generator of discrete rotations (associated to a subgroup of the rotation group) and becomes a finite-dimensional matrix representation of the z -component of the angular momentum.

The notation and language used in this section is that of Quantum Physics, what can be seen as a digression in this numerical look-like paper, but we think that the reasons are obvious.

Let us begin by considering a complete set of quantum states in a space of finite dimension, $|\varphi_j\rangle$, to be determined later. Here, φ_j indicates the j -th eigenvalue of the operator associated to the spatial observable

φ (an angular variable). Now, we ask for the operator that produces a cyclic permutation, within a phase shift factor, of the complete set of states $|\varphi_1\rangle, \dots, |\varphi_N\rangle$, that is, the operator Δ that yields

$$\Delta|\varphi_j\rangle = \begin{cases} e^{i\gamma_{j+1}}|\varphi_{j+1}\rangle, & j \neq N, \\ e^{i\gamma_1}|\varphi_1\rangle, & j = N. \end{cases}$$

Therefore, the representation of Δ in the φ -basis is the matrix of elements $\langle\varphi_j|\Delta|\varphi_k\rangle = \Delta_{jk}$ given by

$$(10) \quad (\Delta_{jk}) = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & e^{i\gamma_1} \\ e^{i\gamma_2} & 0 & 0 & \cdots & 0 & 0 \\ 0 & e^{i\gamma_3} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & e^{i\gamma_N} & 0 \end{pmatrix},$$

yielding that

$$(11) \quad \Delta^N = e^{i\Gamma} 1,$$

where $\Gamma = \sum_{j=1}^N \gamma_j$, and 1 is the identity matrix of dimension N . Since the determinant of Δ is

$$\det \Delta = (-1)^{N+1} e^{i\Gamma},$$

Δ represents a proper rotation and generates a finite subgroup of the rotation group if

$$\Gamma = \begin{cases} 2l\pi, & N \text{ odd}, \\ (2l+1)\pi, & N \text{ even}, \end{cases}$$

with l integer. In such a case, (11) becomes

$$(12) \quad \Delta^N = \begin{cases} 1, & N \text{ odd}, \\ -1, & N \text{ even}, \end{cases}$$

showing that the matrix set of powers of Δ is a representation of the cyclic group of order N or $2N$ for N odd or even respectively (being a two-valued representation of our finite group of rotations in the latter case). Therefore, every eigenvalue of any power of Δ is a rational root of unity. Let us make clear this point because it is related with the main result of this section. By fixing the phase shifts γ_j , we can write (10) in more tractable forms, but due to (12) it is necessary to consider the cases of N odd or even separately. Thus, we can take the $N \times N$ basic circulant permutation matrix

$$\Delta_{jk} = \begin{cases} \delta_{jN}, & \text{for } j = 1, \\ \delta_{j,k+1}, & \text{for } j \geq 2, \end{cases}$$

for (10) in the odd case, whereas, for N even,

$$\Delta_{jk} = \begin{cases} -\delta_{jN}, & \text{for } j = 1, \\ \delta_{j,k+1}, & \text{for } j \geq 2. \end{cases}$$

It is not difficult to see that the characteristic polynomial of Δ in the variable λ is $(-\lambda)^N + 1 = 0$ for any N , and that the N -tuple of components e^{-ika_j}/\sqrt{N} , $k = 1, 2, \dots, N$, is the j -th normalized eigenvector of Δ yielding the eigenvalue $\lambda_j = e^{ia_j}$, where

$$(13) \quad a_j = \frac{2\pi j}{N}, \quad j \in I_N,$$

and

$$I_N = \begin{cases} 0, \pm 1, \pm 2, \dots, \pm n, & N = 2n + 1, \\ \pm 1/2, \pm 3/2, \dots, \pm(2n - 1)/2, & N = 2n. \end{cases}$$

Being Δ unitary, it defines an hermitian matrix A through

$$(14) \quad \Delta = e^{iA}$$

whose eigenvalues are given by (13) (note that the trace of A vanishes) and its eigenvectors, denoted by $|a_j\rangle$, are those of Δ . Therefore, the unitary matrix diagonalizing simultaneously Δ and A is the one with entries

$$(15) \quad \langle \varphi_k | a_j \rangle = \frac{1}{\sqrt{N}} e^{-ika_j}, \quad k, j = 1, 2, \dots, N.$$

In the usual quantum case A becomes proportional to the angle of rotation times L_z . To find a discrete analogue relation we need to calculate the elements of A in the φ -basis. This can be made through

$$A_{jk} = \langle \varphi_j | A | \varphi_k \rangle = \sum_{l=1}^N \langle \varphi_j | a_l \rangle a_l \langle a_l | \varphi_k \rangle = \frac{2\pi}{N^2} \sum_{l \in I_N} l e^{-i(j-k)a_l}.$$

Note that the diagonal elements vanish all of them. For $N = 2n + 1$ we have

$$A_{jk} = -\frac{4\pi}{N^2} i \sum_{l=1}^n l \sin \frac{2\pi l(j-k)}{N},$$

whereas for $N = 2n$,

$$A_{jk} = -\frac{4\pi}{N^2} i \sum_{l=1}^n (l - 1/2) \sin \frac{2\pi(l - 1/2)(j-k)}{N}.$$

These sums can be calculated easily [9] and, for N odd or even, they become

$$(16) \quad A_{jk} = \langle \varphi_j | A | \varphi_k \rangle = \begin{cases} 0, & j = k, \\ \frac{i(-1)^{j+k}\pi/N}{\sin \frac{\pi(j-k)}{N}}, & j \neq k. \end{cases}$$

We proceed now to establish a relation between A and a N -dimensional matrix representation of the derivative of trigonometric polynomials. We choose the odd case $N = 2n + 1$ first.

3.1 Odd case

Let τ_n be the space of trigonometric polynomials of degree at most n . It is well known (see for example [10]) that any trigonometric polynomial $f \in \tau_n$ can be uniquely determined by its values at $2n + 1$ arbitrary points $-\pi < x_1 < x_2 < \dots < x_{2n+1} \leq \pi$, (we change our notation for simplicity) through the formula

$$f(x) = \sum_{k=1}^{2n+1} f(x_k) \frac{t_k(x)}{t_k(x_k)},$$

where the polynomials $t_k \in \tau_n$ are given by

$$(17) \quad t_k(x) = \prod_{l \neq k}^{2n+1} \sin \frac{(x - x_l)}{2}.$$

To reach our goal we need to calculate $\frac{df(x)}{dx}$ at the nodes. The differentiation of (17) and algebraic manipulation of the result yields

$$t'_k(x_j) = \begin{cases} t'(x_k) \sum_{l=1}^{2n+1} \cot \frac{(x_k - x_l)}{2}, & j = k, \\ t'(x_j) \csc \frac{(x_j - x_k)}{2}, & j \neq k, \end{cases},$$

where

$$t(x) = t_k(x) \sin \frac{(x - x_k)}{2} = \prod_{l=1}^{2n+1} \sin \frac{(x - x_l)}{2}.$$

Therefore, $f'(x_j)$ takes the form

$$(18) \quad f'(x_j) = \frac{1}{2} t'(x_j) \sum_{k=1}^{2n+1} \frac{f(x_k)}{\sin \frac{(x_j - x_k)}{2} t'(x_k)} + \frac{1}{2} f(x_j) \sum_{k=1}^{2n+1} \cot \frac{(x_j - x_k)}{2}.$$

Note that $f'(x)$ is again an element of τ_n and that this equation has the structure of (4) with the definitions

$$D = D_\varphi = T \tilde{D} T^{-1},$$

$$(19) \quad \tilde{D}_{ij} = \begin{cases} \sum_{l=1}^N \frac{1}{2} \cot \frac{(x_i - x_l)}{2}, & i = j, \\ \frac{1}{2} \csc \frac{(x_i - x_j)}{2}, & i \neq j, \end{cases} \quad T_{ij} = t'(x_i) \delta_{ij}, \quad i, j = 1, N.$$

Let choose the nodes such that

$$(20) \quad x_j = -\pi + \frac{2\pi j}{N}, \quad j = 1, 2, \dots, N.$$

Then, it is not difficult to see that regardless the parity of N , the product (17) and the sum given by \tilde{D}_{jj} , evaluated at (20), satisfy the equations

$$\frac{t_j(x_j)}{t_k(x_k)} = \frac{t'(x_j)}{t'(x_k)} = (-1)^{j+k},$$

and

$$\tilde{D}_{jj} = \sum_{k=1}^N \cot \frac{(j - k)\pi}{N} = 0, \quad j = 1, 2, \dots, N.$$

Therefore, substituting these expressions in (18) and taking into account (16), we obtain for this choice of nodes and $N = 2n + 1$,

$$(21) \quad A = i \frac{2\pi}{N} D_\varphi = -\frac{2\pi}{N} L_z,$$

where we have defined the N -dimensional matrix L_z as

$$(22) \quad L_z = -iD_\varphi$$

(we take $\hbar = 1$). Therefore, the equation (14) for the discrete rotation operator Δ becomes

$$(23) \quad \Delta = e^{-\frac{2\pi}{N}D_\varphi} = e^{-i\epsilon L_z},$$

where $\epsilon = 2\pi/N$. Like it comes out in the continuum case, the argument of the exponential is proportional to the angle of rotation (in this case ϵ) times the derivative D_φ . Thus, the interpretation of L_z given by (22) as generator of discrete rotations follows immediately. On account of (21), (13) and (15), L_z has the $2n+1$ eigenvalues

$$\{-n, -n+1, \dots, -1, 0, 1, \dots, n-1, n\},$$

and the normalized eigenvectors $|m\rangle$, $m = -n, \dots, n$ whose components, in the φ -basis are

$$\langle \varphi_k | m \rangle = \frac{1}{\sqrt{N}} e^{-im\varphi_k},$$

where $\varphi_k = k\epsilon$, $k = 1, 2, \dots, N$.

The fact that the quantum rule for the z -component of the angular momentum can be projected in a finite-dimensional space maintaining the form it has in the continuum case (a consequence of the use of D_φ as a projection of $\frac{d}{d\varphi}$), reinforces the possibility of the construction of a finite-dimensional algebra for Quantum Mechanics as it appears in other problems [11]–[12].

We consider now the case $N = 2n$, but before we have an important remark. According to the uniqueness of the representation of trigonometric polynomials in terms of the Dirichlet kernel evaluated at differences of (20) (see for example [10]) we have that D_φ equals to $(2n+1)/2$ times the derivative of the Dirichlet kernel evaluated at $x_j - x_k$. On the other hand, it should be pointed out the dependence of the explicit form of the matrix representation of $\frac{d}{d\varphi}$ on the type of projection functions; this means that it is possible to construct other matrices representing the derivative $\frac{d}{d\varphi}$, if we restrict the points to be in $(0, \pi]$ and project on the cosine polynomials.

3.2. Even case

Essentially, the case of $N = 2n$ differs from the odd case only by the space of functions where the projection takes place. Let us begin by considering a function of the form

$$(24) \quad g(x) = \sin(x/2)f(x),$$

where $f \in \tau_{n-1}$. Let $-\pi < x_1^* < x_2^* < \dots < x_{2n-1}^* \leq \pi$ be $N-1$ arbitrary points, different from zero. We can interpolate f at these nodes to yield

$$g(x) = \sum_{k=1}^{N-1} f(x_k^*) \frac{\sin(x/2)t_k^*(x)}{t_k^*(x_k^*)} = \sum_{k=1}^{N-1} [\sin(x_k^*/2)f(x_k^*)] \frac{\sin(x/2)t_k^*(x)}{\sin(x_k^*/2)t_k^*(x_k^*)},$$

that is,

$$(25) \quad g(x) = \sum_{k=1}^{N-1} g(x_k^*) \frac{\sin(x/2)t_k^*(x)}{\sin(x_k^*/2)t_k^*(x_k^*)}.$$

The functions $t_k^*(x)$ are Gaussian polynomials, given by a product like (17) at the $N-1$ nodes x_j^* . Now, let us consider the set of points formed by zero and x_j^* , $j = 1, 2, \dots, N-1$, and denote them by x_j , $j = 1, 2, \dots, 2n$.

Let $t_k(x)$ be the corresponding basic interpolatory polynomials. Then, taking into account that $g(0) = 0$, (25) becomes

$$(26) \quad g(x) = \sum_{k=1}^{2n} g(x_k) \frac{t_k(x)}{t_k(x_k)},$$

and we have an interpolation formula for functions of the form (24) at the points x_j . Therefore, most of the reasonings made in the odd case can be applied to (26) to yield a formula similar to (18) for $g(x)$, so that, for $2n$ points given by any $2n - 1$ different points of $(-\pi, \pi]$ and zero, the matrix

$$(27) \quad D = D_\varphi = T \tilde{D} T^{-1},$$

with the definitions (19) is an exact representation of the derivative of functions given by (24). Moreover, taking into account that $\cos x/2 = \sin[(x + \pi)/2]$ and that π can be taken as one of our nodes and that this function vanishes just at $x = \pi$, we can manipulate the function $h(x) = \cos(x/2)f(x)$ in the same form as we did with (24) to conclude that the k -th power of (27), constructed with a set of $2n$ distinct points of $(-\pi, \pi]$ that includes zero and π , is a $2n$ -dimensional matrix projection of the k -th derivative on the subspace of functions of the type

$$e^{ix/2} f(x),$$

where $f \in \tau_{n-1}$. Now, if we restrict these nodes to be equidistant as in (20), the same formulas (21)-(23) for the relations between A , D_φ , L_z , and Δ are yielded, but now for $N = 2n$. This case makes up a two-valued or spin representation of the finite group of rotations.

Using the same definitions of the preceding case, we have that L_z has the $2n$ eigenvalues

$$\{-(2n-1)/2, -(2n-3)/2, \dots, -1/2, 1/2, \dots, (2n-3)/2, (2n-1)/2\},$$

and the normalized eigenvectors $|m\rangle$, $m = -(2n-1)/2, \dots, (2n-1)/2$ are given again by

$$\langle \varphi_k | m \rangle = \frac{1}{\sqrt{N}} e^{-im\varphi_k},$$

where $\varphi_k = k\epsilon$, $k = 1, 2, \dots, N$.

To end this section let us remark that the validity of formulas (21)-(23) for both N odd and even shows one discrete formulation of rotations in terms of a finite-dimensional matrix representation of the derivative of certain periodic functions that can be associated, according to quantum postulates, to one component of the angular momentum operator projected in \mathbb{C}^N , giving thus, a finite subgroup of the rotation group that shares some of the properties of the full group.

4. The numerical eigenproblem of L^2 .

Our purpose in this section is to obtain a finite-dimensional matrix representation of the angular momentum eigenproblem of a system described by three classical degrees of freedom by applying the results of sections 2 and 3.

As usual, we choose the spherical variables θ and φ to describe the problem. In order to apply the results of section 2, we need two matrices: D_θ of dimension N , and D_φ of dimension M , to represent $d/d\theta$ and $d/d\varphi$ respectively. Since $-\pi < \varphi \leq \pi$ and the functions to represent (the spherical harmonics $Y_n^m(\theta, \varphi)$) are trigonometric polynomials, we will use as matrix D_φ , the one given by (19) with the change of notation $x_j \rightarrow \varphi_j$, where the M points φ_j are given by formula (20):

$$\varphi_j = -\pi + \frac{2\pi j}{M}, \quad j = 1, 2, \dots, M.$$

Concerning the variable θ , we have several alternatives to choose a $N \times N$ matrix for D_θ . Among these, we present only two of them yielding exact results at the nodes. The first one follows the ideas given here and the second is taken from [13].

4.1. A matrix for L^2

Since $0 < \theta \leq \pi$, we can take any set of N distinct points θ_j of $(0, \pi)$ to construct the matrix D_θ according to (19). Besides, the fact that $Y_n^m(\theta, \varphi)$ are defined for integral indexes excludes the use of the spin representations, *i.e.*, the matrices D_φ and D_θ should be constructed with an odd number of points.

Now, according to the results of section 2, the differential eigenvalue problem for $f_s(\theta, \varphi) = Y_n^m(\theta, \varphi)$,

$$\frac{\partial^2 f_s}{\partial^2 \theta} + \cot \theta \frac{\partial f_s}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2 f_s}{\partial^2 \varphi} = -\lambda_s f_s = -n(n+1)f_s,$$

takes the matrix form

$$(28) \quad \mathbf{L}^2 \mathbf{f}_s^* = \lambda_s^* \mathbf{f}_s^*, \quad s = 1, 2, \dots, NM,$$

where \mathbf{L}^2 is the $NM \times NM$ matrix given by

$$(29) \quad \mathbf{L}^2 = -[\mathbf{D}_\theta^2 + \cot(\theta)\mathbf{D}_\theta + \sin^{-2}(\theta)\mathbf{D}_\varphi^2],$$

$\mathbf{f}_s^* \in \mathbb{C}^{NM}$ and λ_s^* is in general a complex number. The matrices of (29) are given by

$$\theta = 1_M \otimes \Theta, \quad \mathbf{D}_\theta = 1_M \otimes D_\theta, \quad \mathbf{D}_\varphi = D_\varphi \otimes 1_N,$$

where Θ is a diagonal matrix with entries $\Theta_{jk} = \theta_j \delta_{jk}$, and 1_K is the identity matrix of dimension K . Thus, (29) can be rewritten as

$$(30) \quad -\mathbf{L}^2 = 1_M \otimes [D_\theta^2 + \cot(\Theta)D_\theta] + D_\varphi^2 \otimes \sin^{-2}(\Theta).$$

Since $Y_n^m(\theta, \varphi)$ is the (tensor) product of the associated Legendre functions $P_n^m(\theta)$ and $e^{im\theta}$ and, on the other hand, we know (from the results of section 3) that the degree of the polynomial that can be differentiated through (19) yielding exact values at N nodes (N odd) is at most $(N-1)/2$, formula (28) reproduces exactly the first

$$\sum_{l=0}^{(N-1)/2} (2l+1) = \left(\frac{N+1}{2}\right)^2$$

eigenvalues and the corresponding unnormalized functions $Y_n^m(\theta, \varphi)$ evaluated at the nodes (θ_j, φ_k) , provided $M \geq N$. In this case \mathbf{L}^2 will have necessarily $(N+1)^2/4$ real eigenvalues given by

$$\lambda_s^* = n(n+1),$$

ordered according to

$$s = n^2 + n + m + 1, \quad n = 0, 1, \dots, (N-1)/2, \quad m = -n, -n+1, \dots, n-1, n.$$

The eigenvector \mathbf{f}_s^* corresponding to λ_s^* , has the components f_{rs}^* given by

$$f_{rs}^* = c_{nm} P_n^m(\theta_j) e^{imk\epsilon},$$

where $\epsilon = 2\pi/M$, c_{nm} is a normalization constant, $\theta_j \in (0, \pi)$, and the relation between r , j and k , is given by (6).

It is possible to choose the θ -nodes in such a way that \mathbf{L}^2 becomes a positive semidefinite matrix (save to a similarity transformation). To see this, note that $-D_\varphi^2$ is positive semidefinite whereas $\sin^{-2}(\Theta)$ is positive definite since $\theta_j \in (0, \pi)$, $j = 1, 2, \dots, N$. Therefore, according to (30) we only have to find the conditions which make the matrix

$$(31) \quad T_\theta^{-1} L_\theta^2 T_\theta = -\tilde{D}_\theta^2 - \cot(\Theta) \tilde{D}_\theta$$

positive semidefinite. To this end, let us separate the main diagonal of D_θ by writing

$$D_\theta = T_\theta D^* T_\theta^{-1} + d,$$

where

$$D_{ij}^* = \begin{cases} 0, & i = j, \\ \frac{1}{2} \csc \frac{(\theta_i - \theta_j)}{2}, & i \neq j, \end{cases} \quad d_{ij} = \delta_{ij} \sum_{l=1}^N \frac{1}{2} \cot \frac{(\theta_i - \theta_j)}{2}$$

[cf. (19)], and T_θ is given by (19). Thus,

$$(32) \quad L_\theta^2 = -T_\theta [D^{*2} + D^* d + d D^* + d^2 + \cot(\Theta) D^* + \cot(\Theta) d] T_\theta^{-1}.$$

If we can find points θ_j such that $d = -\cot(\Theta)/2$, i.e.,

$$(33) \quad \sum_{l=1}^N \cot \frac{(\theta_j - \theta_l)}{2} = -\cot(\theta_j)$$

[cf. (3)], equation (32) becomes

$$L_\theta^2 = T_\theta (-D^{*2} + d D^* - D^* d + d^2) T_\theta^{-1} = T_\theta (-D^* + d)(D^* + d) T_\theta^{-1} = T_\theta \tilde{D}_\theta^t \tilde{D}_\theta T_\theta^{-1},$$

where \tilde{D}_θ^t is the transpose of \tilde{D}_θ . It remains to show that a solution of (33) always exists. Since $\cot x$ is the logarithmic derivative of $\sin x$, Eq. (33) is the condition for a critical point of the function of N variables

$$U(z) = U(z_1, z_2, \dots, z_N) = \prod_{k=1}^N \sin(z_k) \prod_{i>j}^N \sin \frac{(z_i - z_j)}{2},$$

where $0 \leq z_j \leq \pi$, $j = 1, 2, \dots, N$. The existence (and uniqueness) of the solution can be proved along the same lines given in [14]. It is worth to be noticed that the similarity transformation is not essential for an eigenproblem like (28) since the similarity matrices corresponding to θ and φ can be collected into a $NM \times NM$ diagonal matrix \mathbf{S} to write (28) in the form

$$\mathbf{L}_P^2 \mathbf{g}_s = \lambda_s^* \mathbf{g}_s,$$

where $\mathbf{g}_s = \mathbf{S}^{-1} \mathbf{f}_s^*$ and \mathbf{L}_P^2 is positive semidefinite. Thus, if we construct L_θ^2 with the set of nodes satisfying (33), \mathbf{L}^2 is a positive semidefinite matrix (save a similarity transformation), a necessary property from the numerical and physical point of view in any projection scheme.

4.2. Other matrix for L^2

In [13], a matrix representation of the derivative for trigonometric polynomials of definite parity is given and, therefore, it can also be used to construct a representative of (31), yielding a matrix for L^2 with a higher degree of approximation than (29). The cost we have to afford for this is the lacking of simplicity: we can not use a single matrix for $\frac{d}{d\theta}$ to be substituted directly in (31) unless we accept to loose precision in the results (see [13]). According to this scheme, the representation of a differential operator is formed following a given rule where certain matrix \mathbf{D} is involved. Such a matrix is constructed with N arbitrary distinct points $\theta_j \in (0, \pi)$ through a formula similar to (19)

$$\mathbf{D} = \mathbf{D}_\theta = \mathbf{S} \tilde{\mathbf{D}} \mathbf{S}^{-1},$$

$$\tilde{D}_{ij} = \begin{cases} \sum_{l=1}^N \cot(\theta_i - \theta_l), & i = j, \\ \cot(\theta_i - \theta_j), & i \neq j, \end{cases} \quad S_{ij} = \delta_{ij} \prod_{l \neq j}^N \sin(\theta_j - \theta_l).$$

The form that L_θ^2 adopts in this case is

$$(34) \quad L_\theta^2 = -D_\theta^2 - \cot(\Theta)D_\theta + NSOS^{-1},$$

where Θ is again a diagonal matrix with entries $\Theta_{jk} = \theta_j \delta_{jk}$ and O is a projection matrix with ones everywhere, *i.e.*, $O_{jk} = 1$. According to [13], the degree of approximation of (34) is higher than that of (31). While the former yields exact results at N nodes (N odd or even) for trigonometric polynomials (of definite parity) of degree N , the latter produces exact results for polynomials of degree $(N-1)/2$ (N odd). Thus, the use of (34) in (30) gives the matrix

$$(35) \quad -\mathbf{L}^2 = 1_M \otimes [D_\theta^2 + \cot(\Theta)D_\theta - NSOS^{-1}] + D_\varphi^2 \otimes \sin^{-2}(\Theta)$$

with a higher degree of approximation: if N is an odd integer and $M = 2N + 1$, then (35) produces the first

$$\sum_{l=0}^N (2l+1) = (N+1)^2$$

exact eigenvalues (and eigenvectors) while (30) yields only the first $(N+1)^2/4$ for the same values of N and M .

5. Final remarks

Summarizing, we have found a finite-dimensional representation of the square of quantum angular momentum with the following properties:

1. The coordinate representation of the z -component of the angular momentum operator is maintained in this discrete scheme and the projection of L_z is the generator of a finite subgroup of the group of rotations.
2. The projection of L^2 is given in terms of finite-dimensional representations of the partial derivatives according to the well-known formula for L^2 .
3. The spectrum of this projection contains the first eigenvalues of L^2 (counting the degeneracy) in such a form that the whole spectrum of L^2 can be reobtained when the number of nodes tends to infinity.
4. The eigenvectors of this projection, corresponding to the exact eigenvalues of L^2 , can be converted into the exact eigenfunctions through an interpolation at the nodes. Again, this process yields the complete set of eigenfunctions of L^2 when the dimension of \mathbf{L}^2 tends to infinity.

Finally, we note that these properties makes \mathbf{L}^2 suitable for numerical applications to quantum problems as it will be shown in a subsequent work.

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